



## wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 08:35 AM EDT

PDB ID : 8TQW  
EMDB ID : EMD-41565  
Title : Structure of human transcriptional Mediator complex  
Authors : Chen, S.F.; Chao, T.C.; Kim, H.J.; Tang, H.C.; Khadka, S.; Li, T.; Murakami, K.; Boyer, T.G.; Tsai, K.L.  
Deposited on : 2023-08-08  
Resolution : 8.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

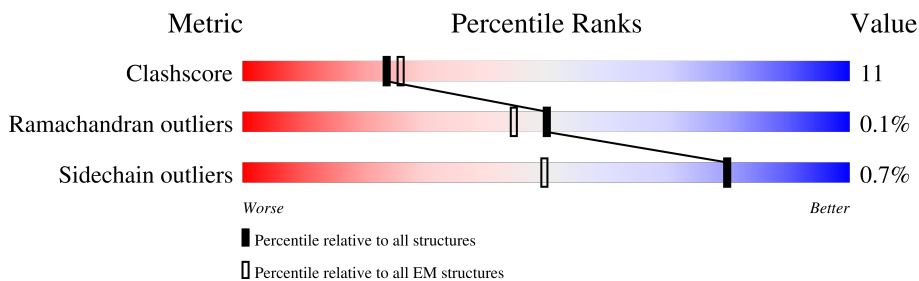
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









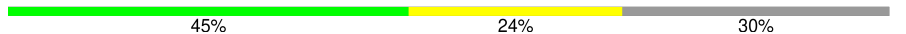














Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	311	68% 18% 14%
2	1	178	33% 22% 44%
3	2	200	48% 10% 42%
4	3	178	52% 16% 31%
5	4	131	57% 29% 14%
6	A	1581	19% 11% 70%
7	B	20	65% 35%
8	D	270	36% 21% 41%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F	246	
10	G	233	
11	H	268	
12	I	146	
13	J	135	
14	K	117	
15	N	1454	
16	O	788	
17	P	877	
18	Q	651	
19	R	208	
20	S	244	
21	T	212	
22	U	144	
23	V	200	
24	W	1368	
25	X	989	
26	a	464	
27	b	283	
28	c	2177	
29	d	2174	

## 2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 83816 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	267	2159	1373	384	390	12	0	0

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	99	817	511	143	160	3	0	0

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	115	899	563	155	172	9	0	0

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	122	1022	639	187	189	7	0	0

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	113	986	642	171	168	5	0	0

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	467	3578	2278	613	663	24	0	0

- Molecule 7 is a protein called Unknown Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	B	20	100	60	20	20	0	0

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	158	1268	791	228	243	6	0	0

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	166	1363	882	234	242	5	0	0

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	161	1348	856	239	243	10	0	0

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	H	181	1422	888	250	280	4	0	0

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	73	605	382	107	110	6	0	0

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	122	840	527	151	159	3	0	0

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	K	112	879	537	163	175	4	0	0

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	N	1017	7772	4958	1365	1407	42	0	0

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	O	157	1226	783	213	223	7	0	0

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	P	753	5875	3742	1008	1077	48	0	0

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Q	546	4319	2732	773	794	20	0	0

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	R	191	1532	971	270	276	15	0	0

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	S	75	517	328	87	100	2	0	0

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	T	193	1499	955	247	280	17	0	0

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	U	121	918	570	153	190	5	0	0

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	V	130	1063	656	181	222	4	0	0

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	W	1334	10774	6967	1827	1909	71	0	0

- Molecule 25 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	X	897	7061	4524	1190	1293	54	0	0

- Molecule 26 is a protein called Cyclin-dependent kinase 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	313	2561	1663	439	442	17	0	0

- Molecule 27 is a protein called Cyclin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	262	2196	1442	358	379	17	1	0

- Molecule 28 is a protein called Mediator of RNA polymerase II transcription subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	1452	11499	7270	2009	2147	73	0	0

- Molecule 29 is a protein called Mediator of RNA polymerase II transcription subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	969	7714	4945	1310	1393	66	0	0

- Molecule 30 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

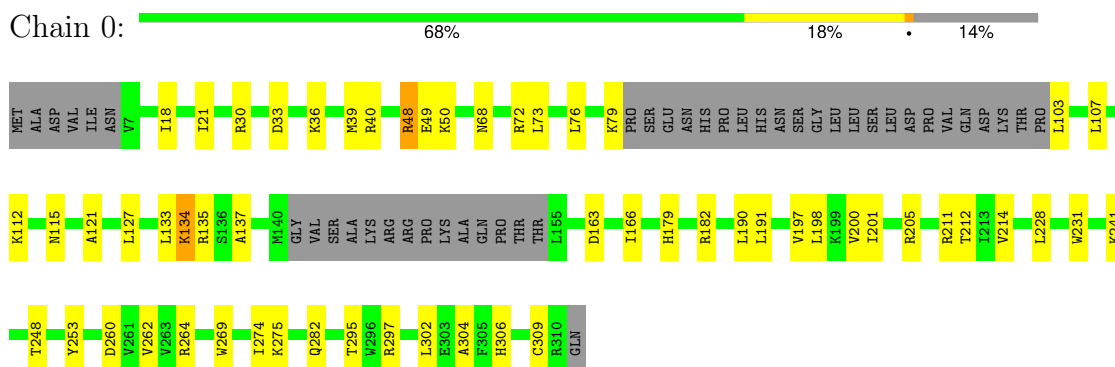
Mol	Chain	Residues	Atoms		AltConf
30	0	1	Total 1	Zn 1	0
30	P	1	Total 1	Zn 1	0
30	c	1	Total 1	Zn 1	0
30	d	1	Total 1	Zn 1	0



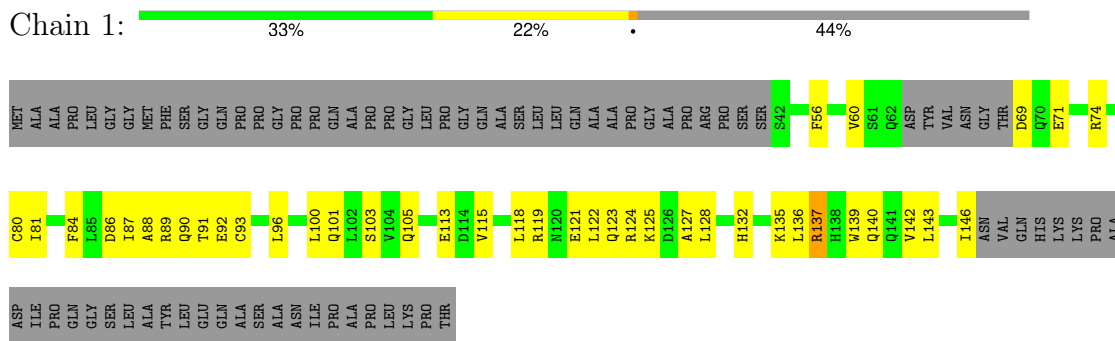
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

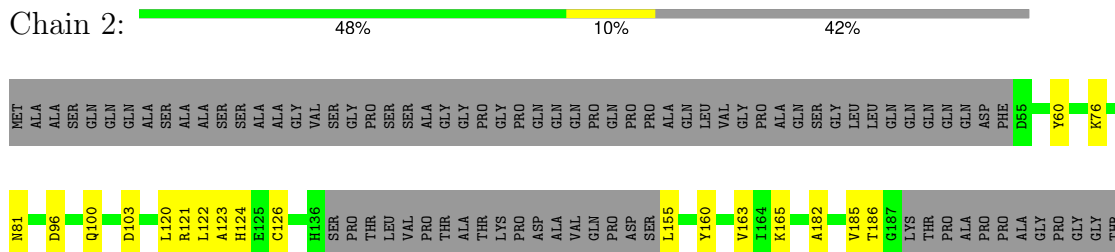
- Molecule 1: Mediator of RNA polymerase II transcription subunit 27



- Molecule 2: Mediator of RNA polymerase II transcription subunit 28



- Molecule 3: Mediator of RNA polymerase II transcription subunit 29

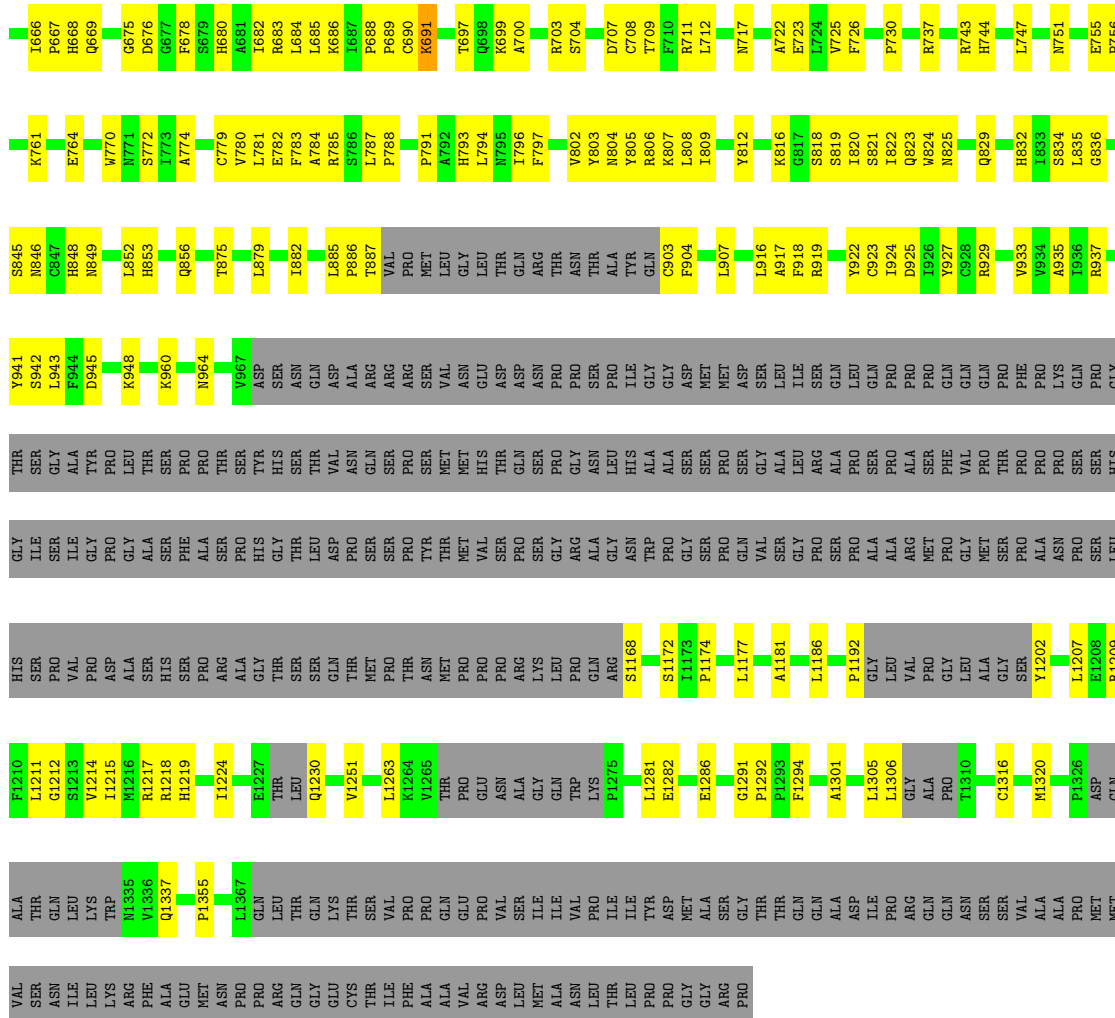




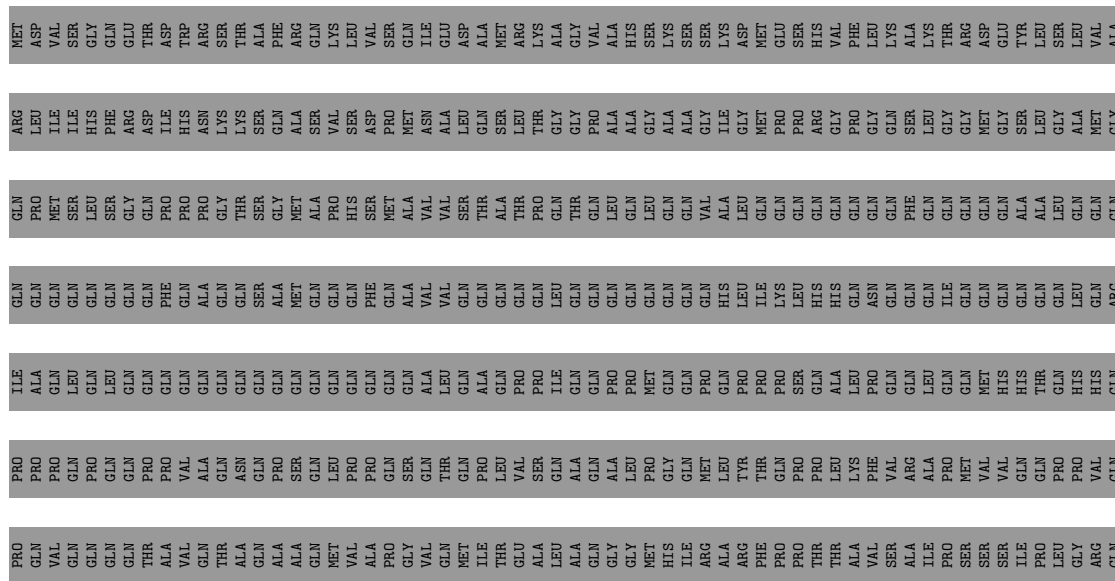




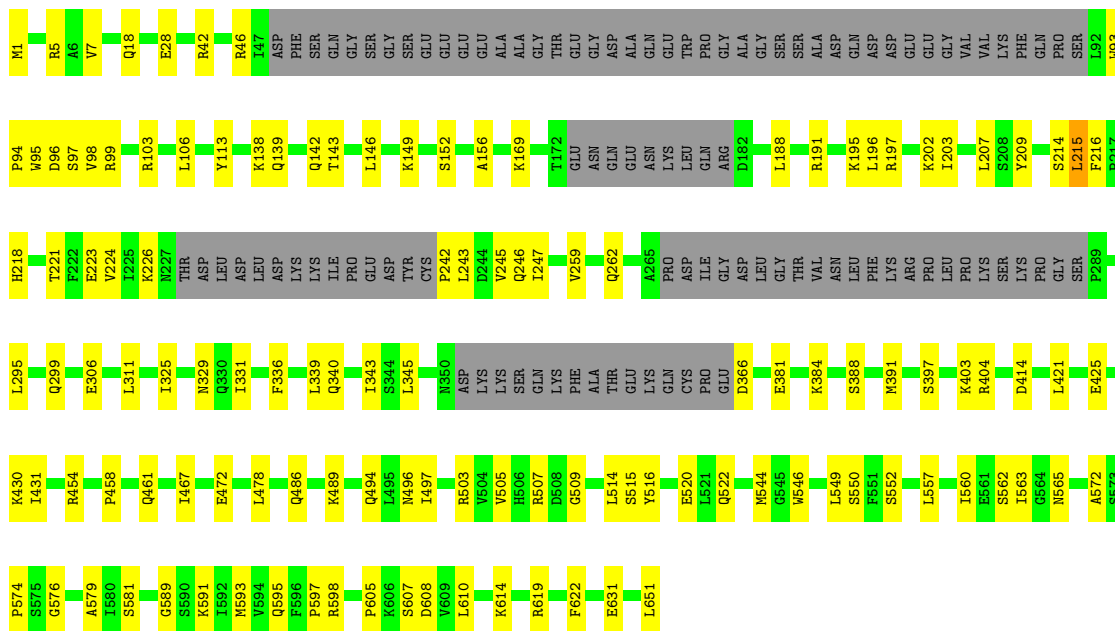




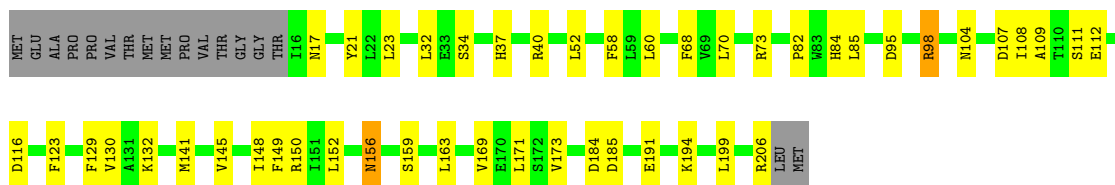
● Molecule 16: Mediator of RNA polymerase II transcription subunit 15



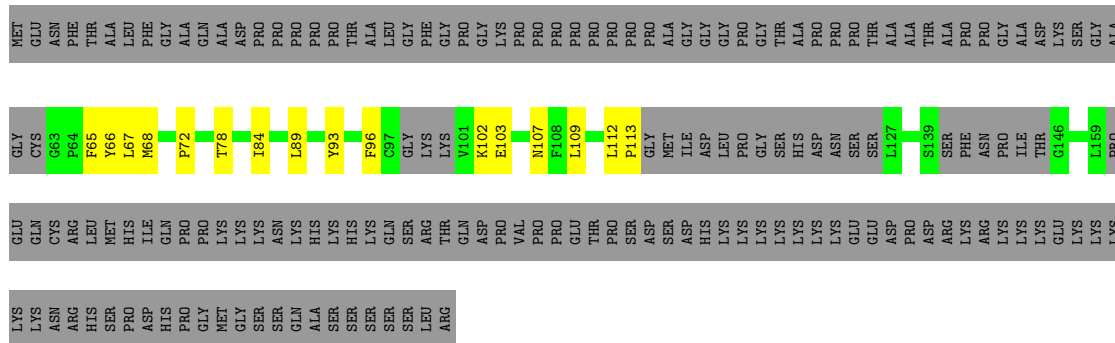




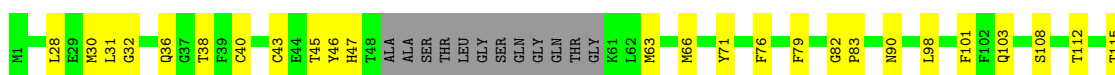
• Molecule 19: Mediator of RNA polymerase II transcription subunit 18



• Molecule 20: Mediator of RNA polymerase II transcription subunit 19

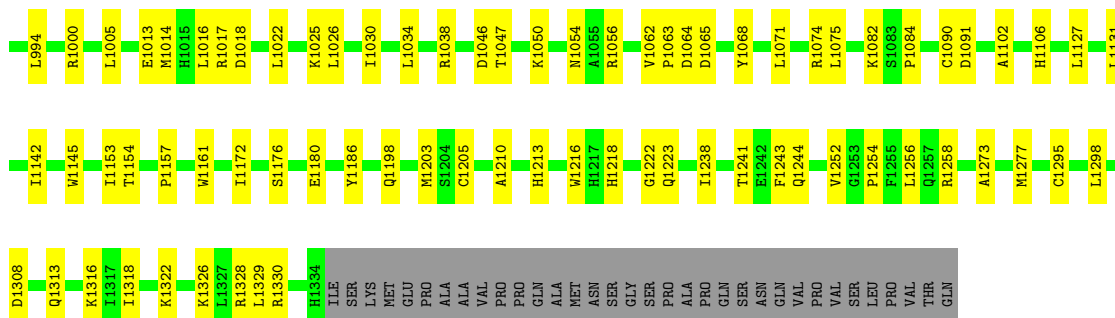


• Molecule 21: Mediator of RNA polymerase II transcription subunit 20

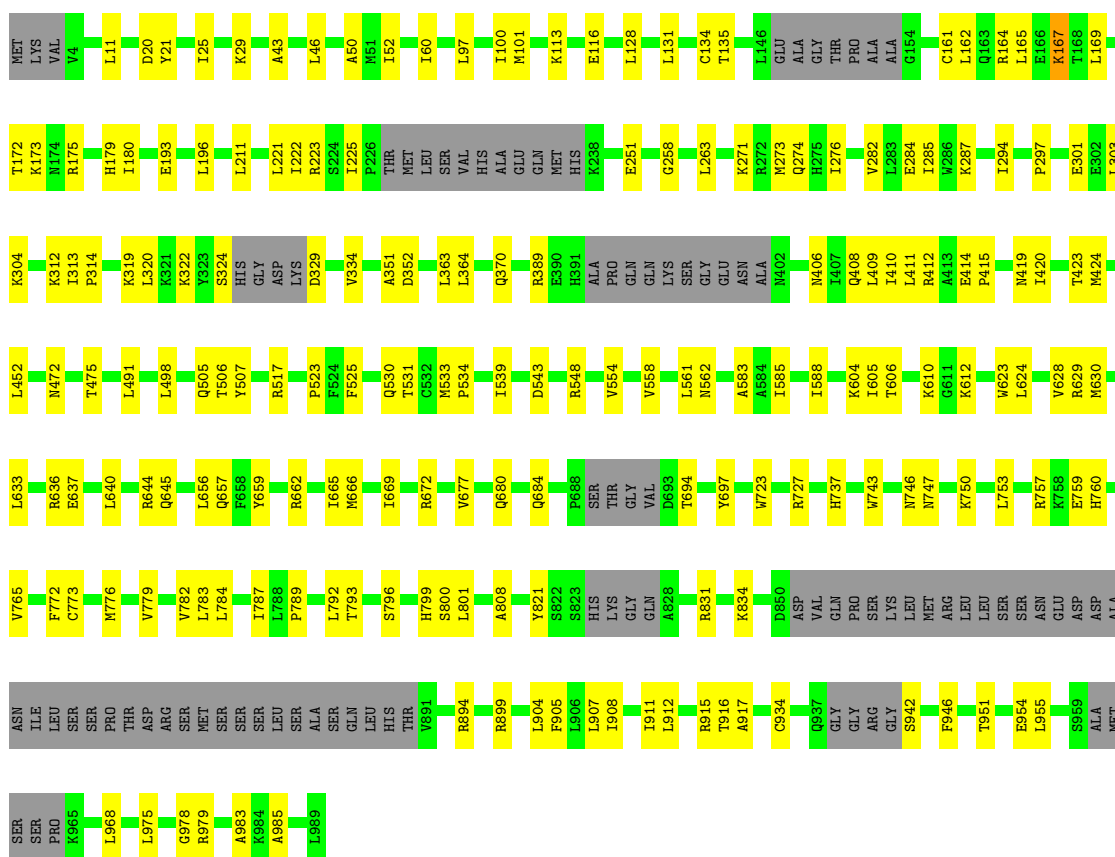




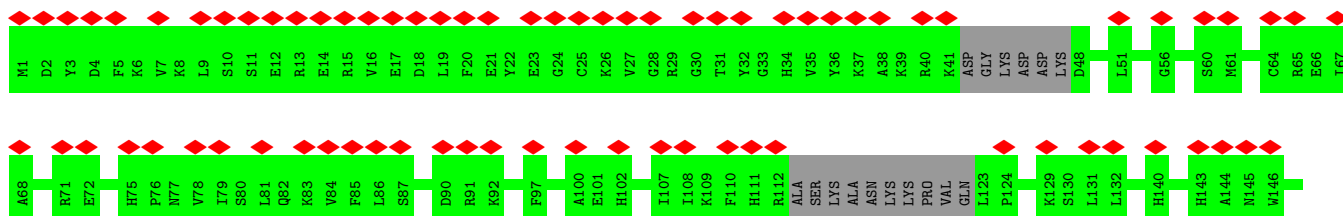
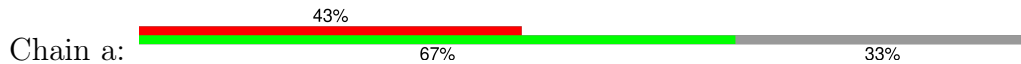


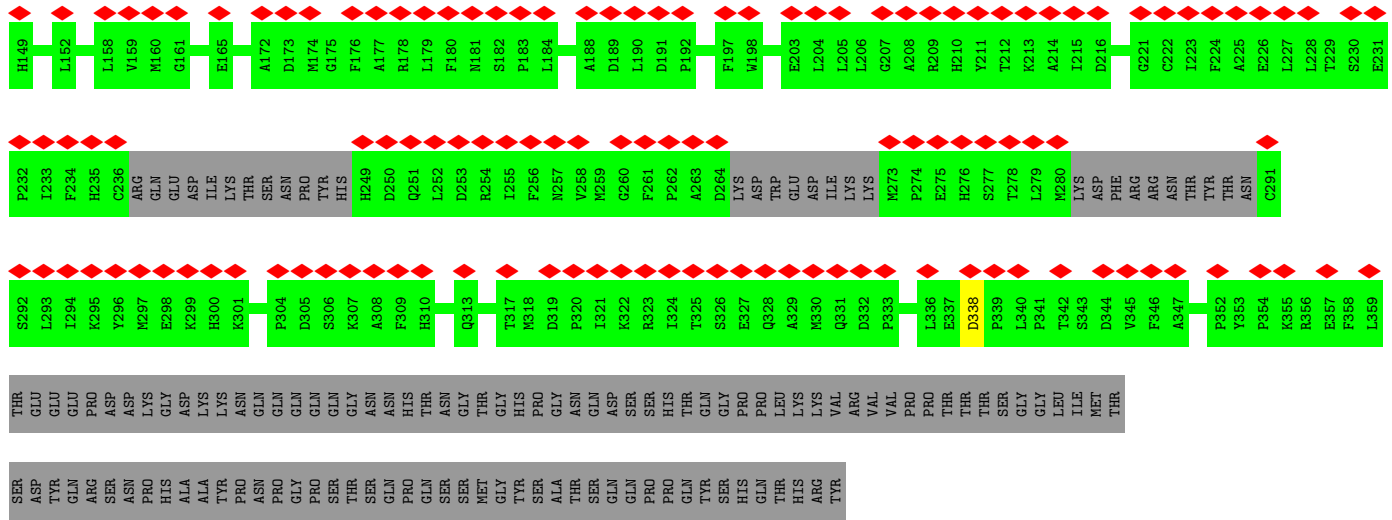


• Molecule 25: Mediator of RNA polymerase II transcription subunit 24

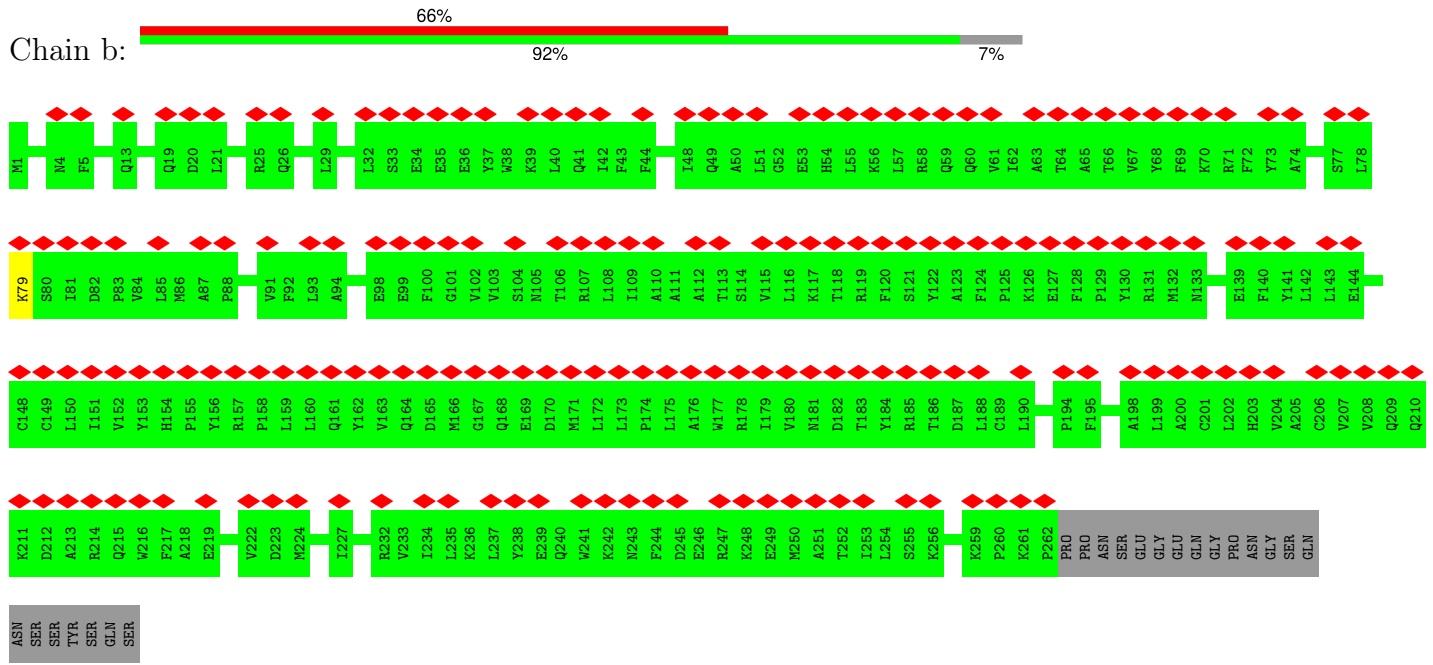


• Molecule 26: Cyclin-dependent kinase 8

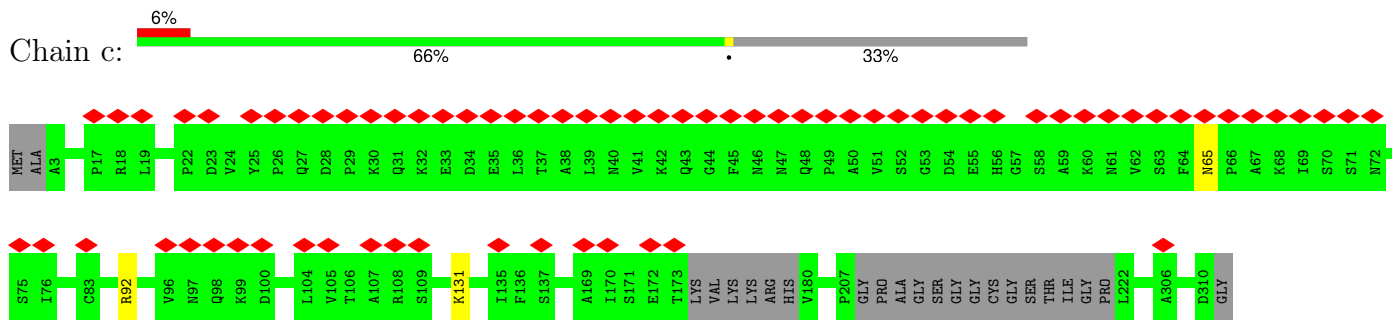


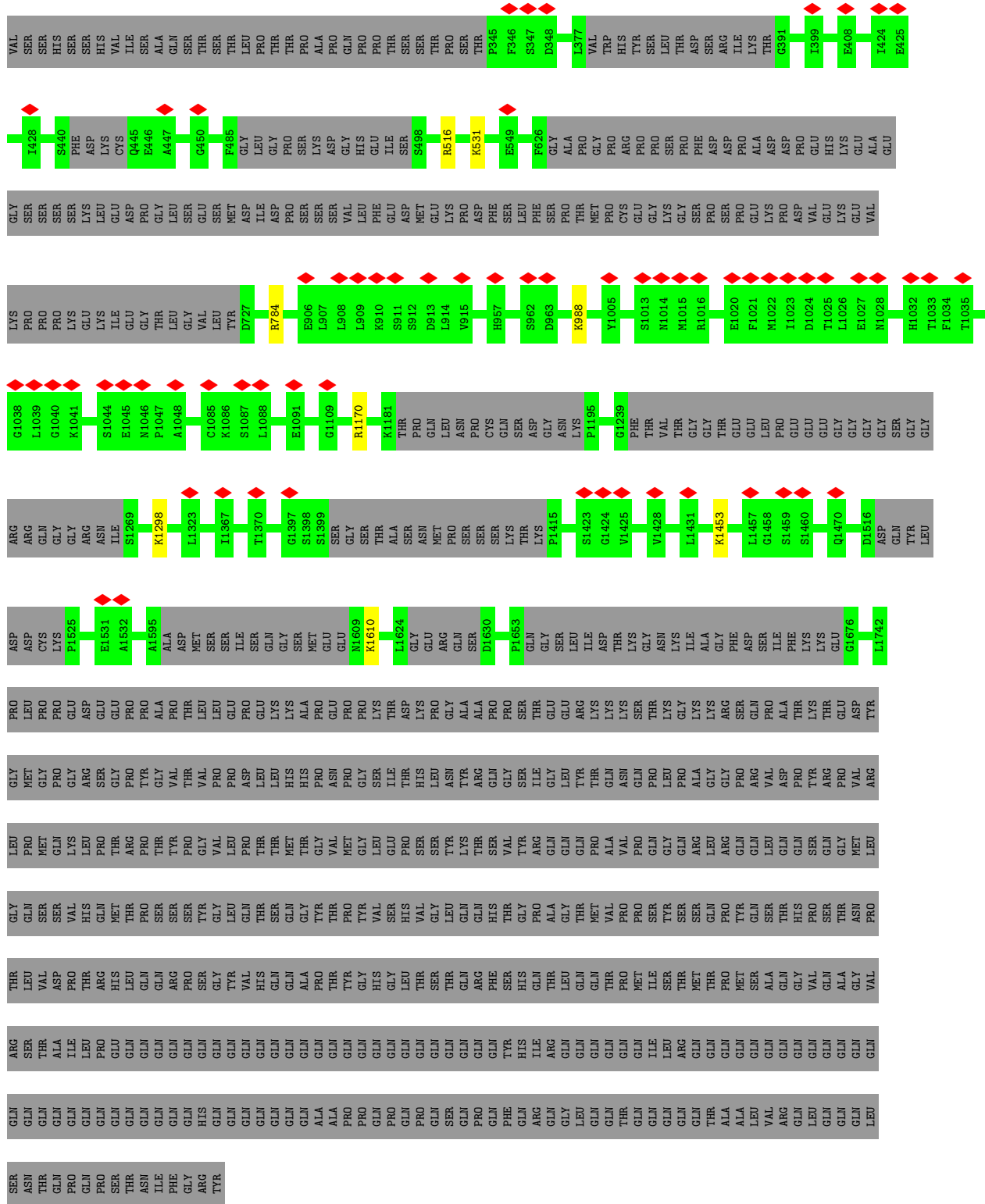


• Molecule 27: Cyclin-C

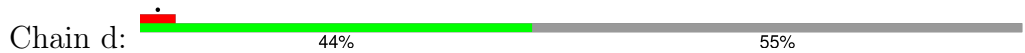


• Molecule 28: Mediator of RNA polymerase II transcription subunit 12





- Molecule 29: Mediator of RNA polymerase II transcription subunit 13







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size ( $\text{\AA}$ )	727.04004, 727.04004, 727.04004	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.272, 2.272, 2.272	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.26	0/2201	0.58	0/2972
2	1	0.35	0/825	0.60	0/1107
3	2	0.26	0/911	0.49	0/1229
4	3	0.25	0/1029	0.61	0/1378
5	4	0.29	0/1013	0.55	0/1364
6	A	0.34	0/3653	0.60	0/4961
8	D	0.29	0/1281	0.61	0/1718
9	F	0.29	0/1400	0.61	0/1902
10	G	0.30	0/1374	0.61	0/1847
11	H	0.26	0/1441	0.59	0/1946
12	I	0.28	0/612	0.68	0/815
13	J	0.28	0/849	0.52	0/1150
14	K	0.25	0/885	0.59	0/1190
15	N	0.32	0/7923	0.60	0/10761
16	O	0.26	0/1261	0.61	0/1731
17	P	0.26	0/6001	0.61	0/8151
18	Q	0.26	0/4400	0.56	0/5941
19	R	0.26	0/1562	0.59	0/2101
20	S	0.28	0/524	0.55	0/709
21	T	0.28	0/1530	0.57	0/2066
22	U	0.26	0/927	0.53	0/1257
23	V	0.25	0/1072	0.54	0/1440
24	W	0.26	0/11056	0.52	0/15023
25	X	0.26	0/7191	0.55	0/9728
26	a	0.27	0/2627	0.56	0/3542
27	b	0.27	0/2253	0.56	0/3051
28	c	0.27	0/11719	0.57	0/15850
29	d	0.26	0/7895	0.56	0/10703
All	All	0.27	0/85415	0.57	0/115633

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	2159	0	2176	37	0
2	1	817	0	818	71	0
3	2	899	0	908	14	0
4	3	1022	0	1054	27	0
5	4	986	0	965	28	0
6	A	3578	0	3522	146	0
7	B	100	0	23	4	0
8	D	1268	0	1305	60	0
9	F	1363	0	1344	22	0
10	G	1348	0	1373	74	0
11	H	1422	0	1440	23	0
12	I	605	0	628	33	0
13	J	840	0	718	34	0
14	K	879	0	886	7	0
15	N	7772	0	7557	349	0
16	O	1226	0	1217	21	0
17	P	5875	0	5968	145	0
18	Q	4319	0	4403	118	0
19	R	1532	0	1542	29	0
20	S	517	0	432	24	0
21	T	1499	0	1484	35	0
22	U	918	0	905	12	0
23	V	1063	0	1051	48	0
24	W	10774	0	10838	194	0
25	X	7061	0	7223	128	0
26	a	2561	0	2578	0	0
27	b	2196	0	2233	0	0
28	c	11499	0	11504	0	0
29	d	7714	0	7627	0	0
30	0	1	0	0	0	0
30	P	1	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	c	1	0	0	0	0
30	d	1	0	0	0	0
All	All	83816	0	83722	1451	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1451 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:375:ASP:CB	15:N:376:PRO:HD3	1.67	1.22
2:1:115:VAL:HG22	4:3:142:ILE:HD11	1.29	1.14
12:I:109:LEU:CD2	12:I:114:GLN:HE21	1.60	1.14
12:I:140:MET:O	22:U:117:LYS:HD3	1.44	1.14
10:G:104:LYS:HD3	20:S:72:PRO:HG3	1.19	1.13

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	261/311 (84%)	250 (96%)	11 (4%)	0	100	100
2	1	95/178 (53%)	92 (97%)	3 (3%)	0	100	100
3	2	111/200 (56%)	107 (96%)	4 (4%)	0	100	100
4	3	114/178 (64%)	112 (98%)	2 (2%)	0	100	100
5	4	111/131 (85%)	106 (96%)	5 (4%)	0	100	100
6	A	455/1581 (29%)	427 (94%)	27 (6%)	1 (0%)	44	78
8	D	154/270 (57%)	148 (96%)	6 (4%)	0	100	100
9	F	162/246 (66%)	148 (91%)	14 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	G	159/233 (68%)	152 (96%)	7 (4%)	0	100	100
11	H	177/268 (66%)	169 (96%)	7 (4%)	1 (1%)	22	60
12	I	69/146 (47%)	66 (96%)	3 (4%)	0	100	100
13	J	120/135 (89%)	119 (99%)	1 (1%)	0	100	100
14	K	110/117 (94%)	108 (98%)	2 (2%)	0	100	100
15	N	995/1454 (68%)	902 (91%)	89 (9%)	4 (0%)	30	68
16	O	153/788 (19%)	143 (94%)	10 (6%)	0	100	100
17	P	743/877 (85%)	689 (93%)	53 (7%)	1 (0%)	48	83
18	Q	534/651 (82%)	497 (93%)	36 (7%)	1 (0%)	44	78
19	R	189/208 (91%)	177 (94%)	12 (6%)	0	100	100
20	S	67/244 (28%)	65 (97%)	1 (2%)	1 (2%)	8	40
21	T	189/212 (89%)	166 (88%)	23 (12%)	0	100	100
22	U	117/144 (81%)	114 (97%)	3 (3%)	0	100	100
23	V	128/200 (64%)	122 (95%)	6 (5%)	0	100	100
24	W	1332/1368 (97%)	1278 (96%)	54 (4%)	0	100	100
25	X	877/989 (89%)	828 (94%)	49 (6%)	0	100	100
26	a	301/464 (65%)	292 (97%)	8 (3%)	1 (0%)	37	73
27	b	261/283 (92%)	258 (99%)	3 (1%)	0	100	100
28	c	1422/2177 (65%)	1359 (96%)	63 (4%)	0	100	100
29	d	923/2174 (42%)	874 (95%)	49 (5%)	0	100	100
All	All	10329/16227 (64%)	9768 (95%)	551 (5%)	10 (0%)	50	83

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	375	ASP
20	S	67	LEU
26	a	338	ASP
11	H	99	VAL
17	P	362	SER

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	241/280 (86%)	238 (99%)	3 (1%)	67	78
2	1	94/152 (62%)	93 (99%)	1 (1%)	70	80
3	2	102/163 (63%)	101 (99%)	1 (1%)	73	82
4	3	116/155 (75%)	116 (100%)	0	100	100
5	4	102/115 (89%)	102 (100%)	0	100	100
6	A	394/1391 (28%)	393 (100%)	1 (0%)	91	92
8	D	139/230 (60%)	134 (96%)	5 (4%)	30	50
9	F	150/223 (67%)	149 (99%)	1 (1%)	81	87
10	G	153/216 (71%)	153 (100%)	0	100	100
11	H	161/225 (72%)	160 (99%)	1 (1%)	84	88
12	I	71/133 (53%)	68 (96%)	3 (4%)	25	46
13	J	66/124 (53%)	62 (94%)	4 (6%)	15	37
14	K	94/98 (96%)	93 (99%)	1 (1%)	70	80
15	N	810/1271 (64%)	808 (100%)	2 (0%)	92	94
16	O	141/697 (20%)	140 (99%)	1 (1%)	81	87
17	P	670/766 (88%)	667 (100%)	3 (0%)	89	91
18	Q	488/577 (85%)	485 (99%)	3 (1%)	84	88
19	R	169/183 (92%)	166 (98%)	3 (2%)	54	71
20	S	43/208 (21%)	43 (100%)	0	100	100
21	T	166/178 (93%)	164 (99%)	2 (1%)	67	78
22	U	98/119 (82%)	97 (99%)	1 (1%)	73	82
23	V	122/173 (70%)	122 (100%)	0	100	100
24	W	1203/1232 (98%)	1200 (100%)	3 (0%)	92	94
25	X	789/864 (91%)	786 (100%)	3 (0%)	89	91
26	a	277/412 (67%)	277 (100%)	0	100	100
27	b	241/258 (93%)	240 (100%)	1 (0%)	89	91
28	c	1282/1916 (67%)	1271 (99%)	11 (1%)	75	83
29	d	869/1918 (45%)	862 (99%)	7 (1%)	79	85
All	All	9251/14277 (65%)	9190 (99%)	61 (1%)	80	87

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	Q	215	LEU
29	d	275	ARG
22	U	92	LYS
29	d	231	LYS
29	d	1359	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
28	c	1729	HIS
29	d	1131	ASN
15	N	909	GLN
15	N	507	GLN
29	d	1137	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

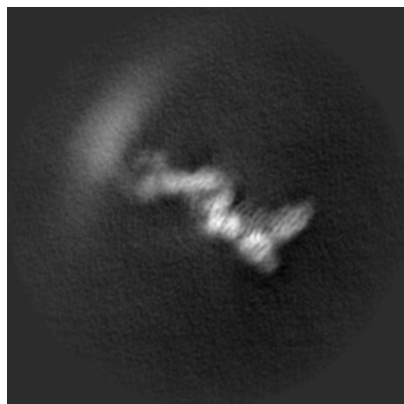
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41565. These allow visual inspection of the internal detail of the map and identification of artifacts.

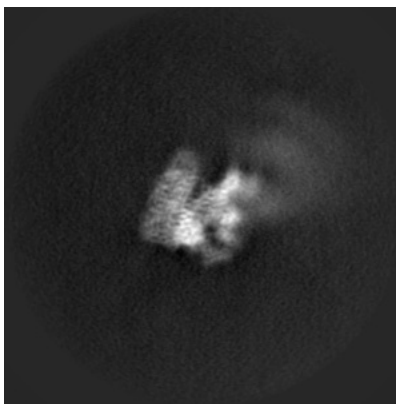
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

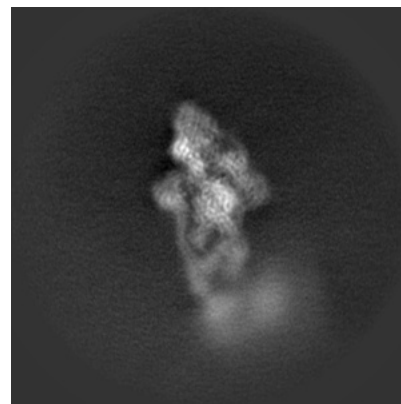
#### 6.1.1 Primary map



X

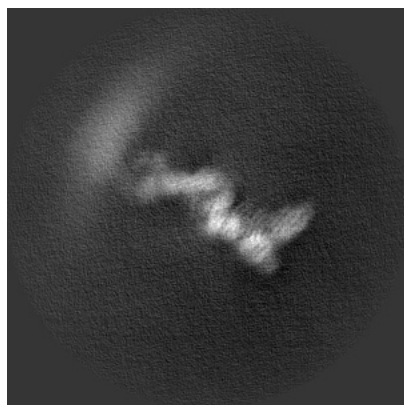


Y

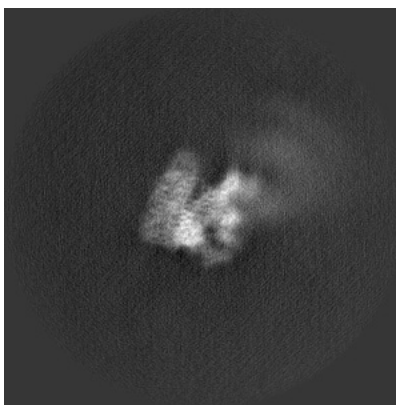


Z

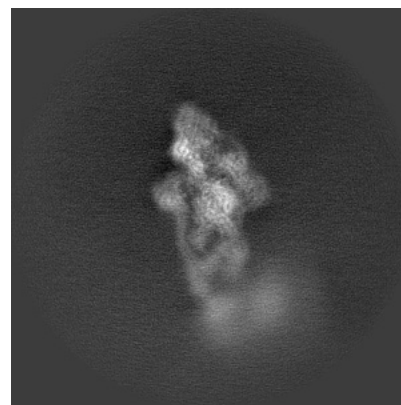
#### 6.1.2 Raw map



X



Y

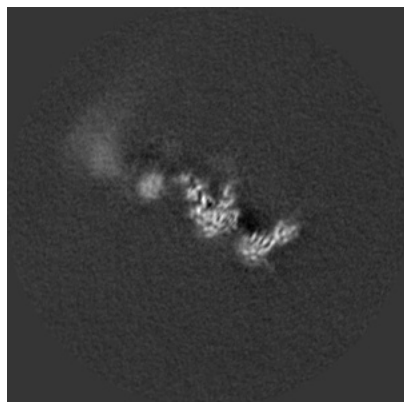


Z

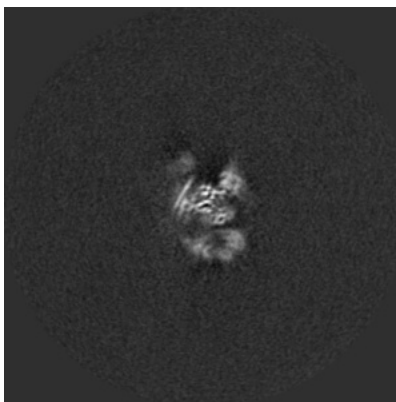
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

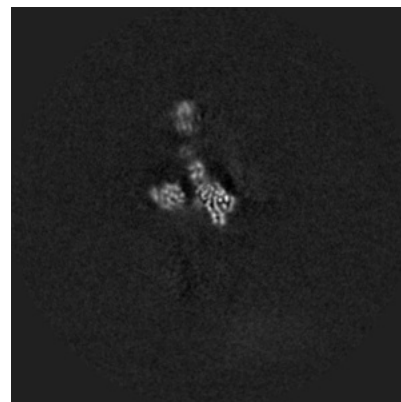
### 6.2.1 Primary map



X Index: 160

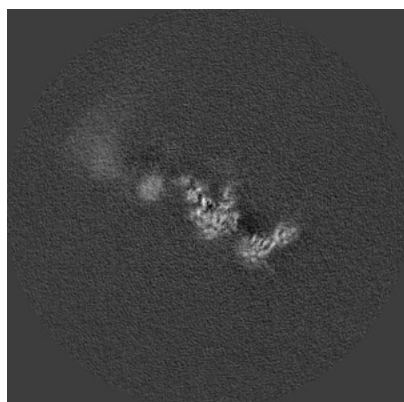


Y Index: 160

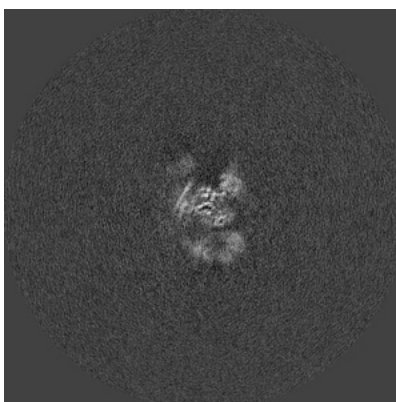


Z Index: 160

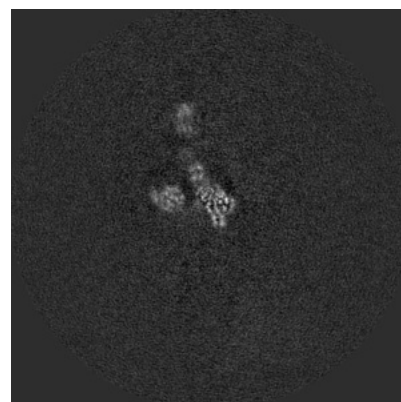
### 6.2.2 Raw map



X Index: 160



Y Index: 160



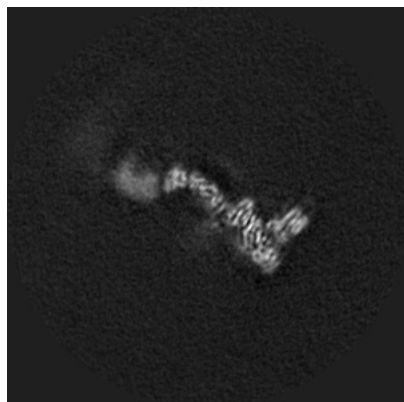
Z Index: 160

The images above show central slices of the map in three orthogonal directions.

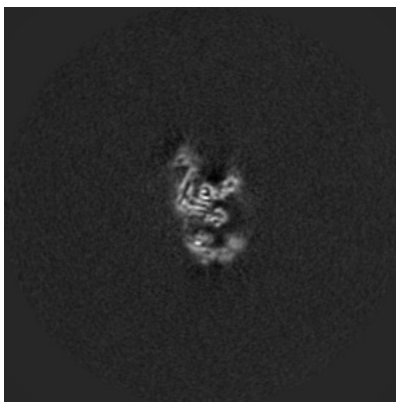


## 6.3 Largest variance slices [i](#)

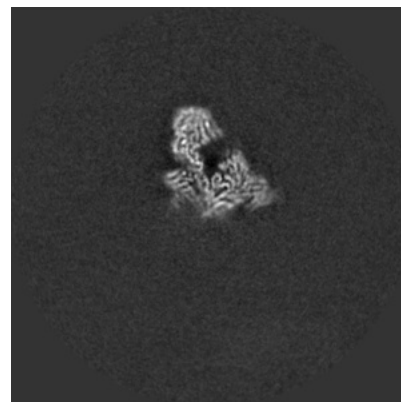
### 6.3.1 Primary map



X Index: 149

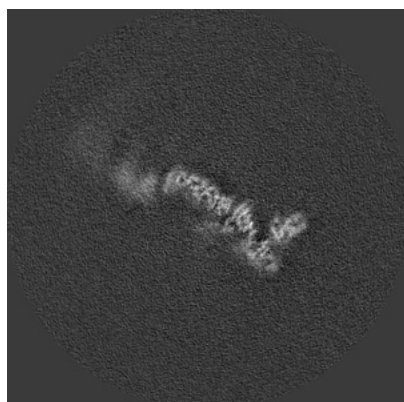


Y Index: 165

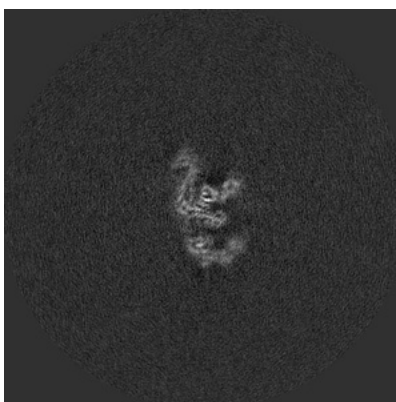


Z Index: 145

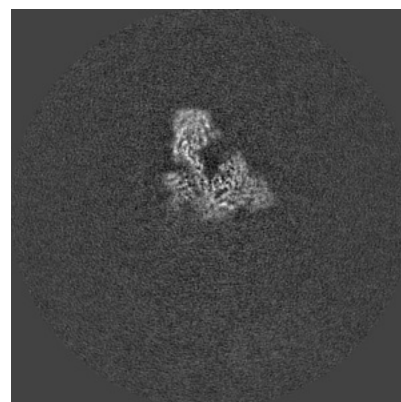
### 6.3.2 Raw map



X Index: 152



Y Index: 166



Z Index: 146

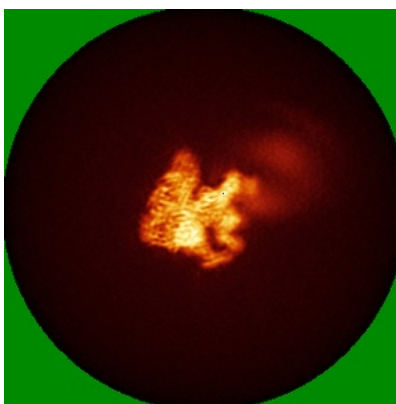
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

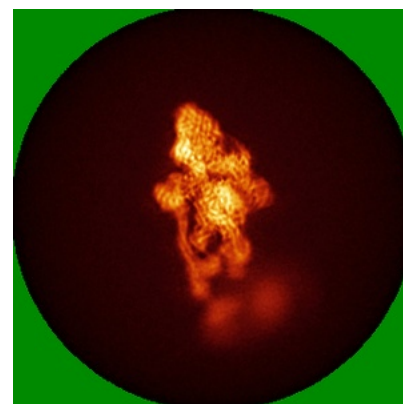
### 6.4.1 Primary map



X

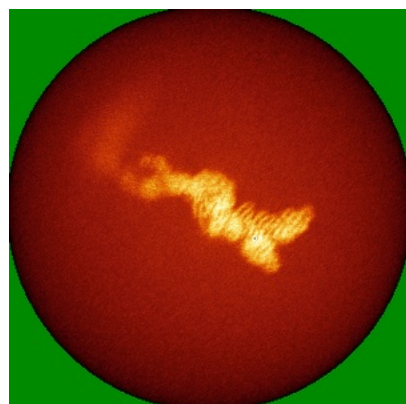


Y

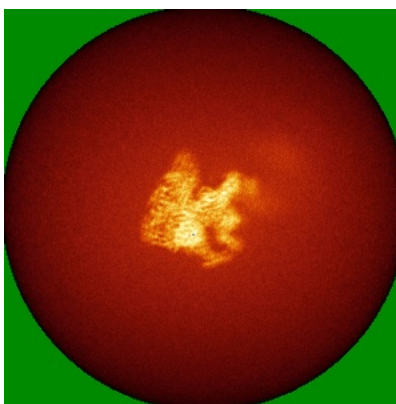


Z

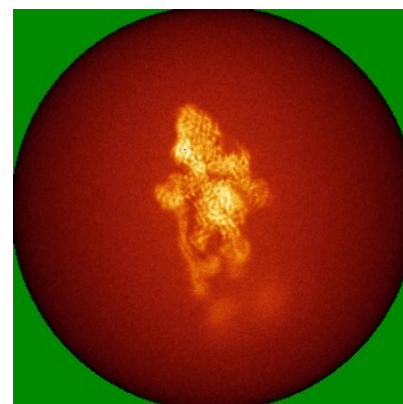
### 6.4.2 Raw map



X



Y

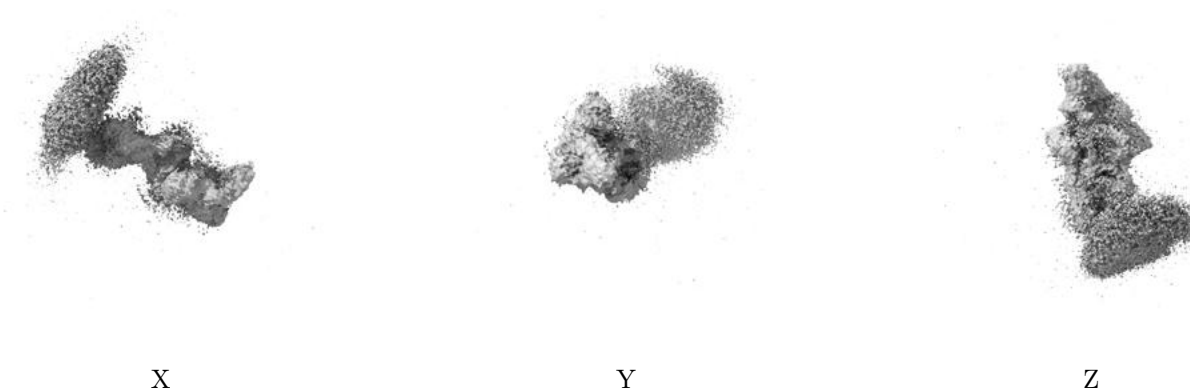


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

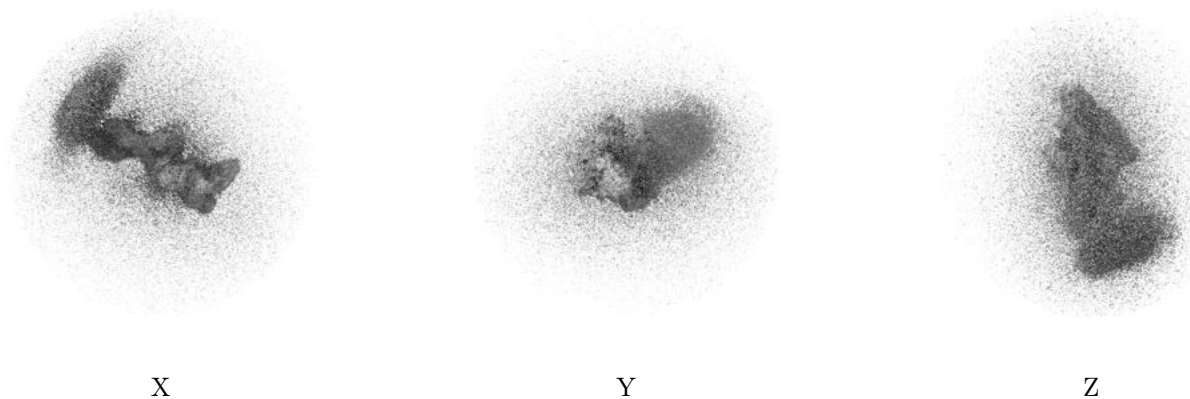
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

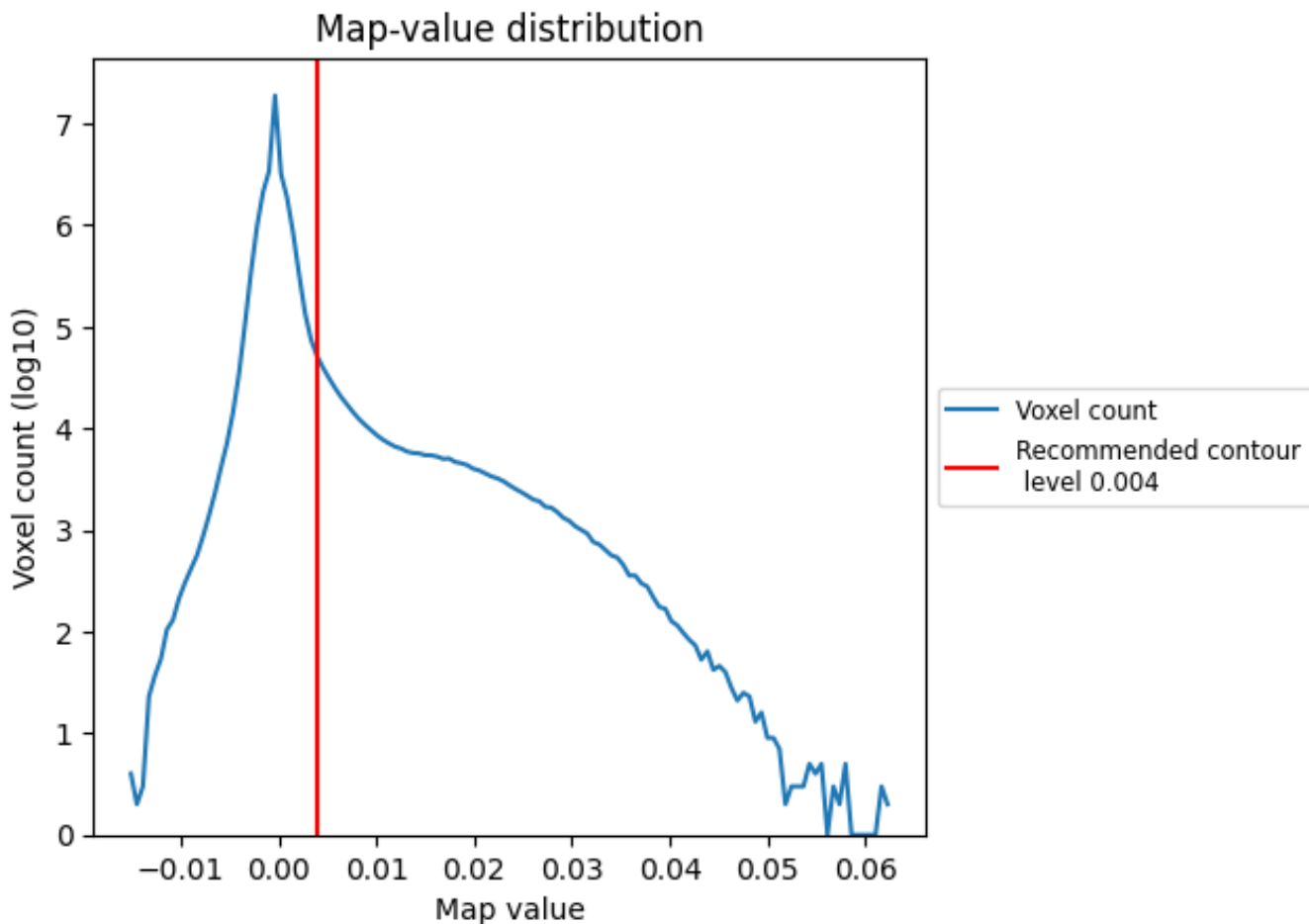
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

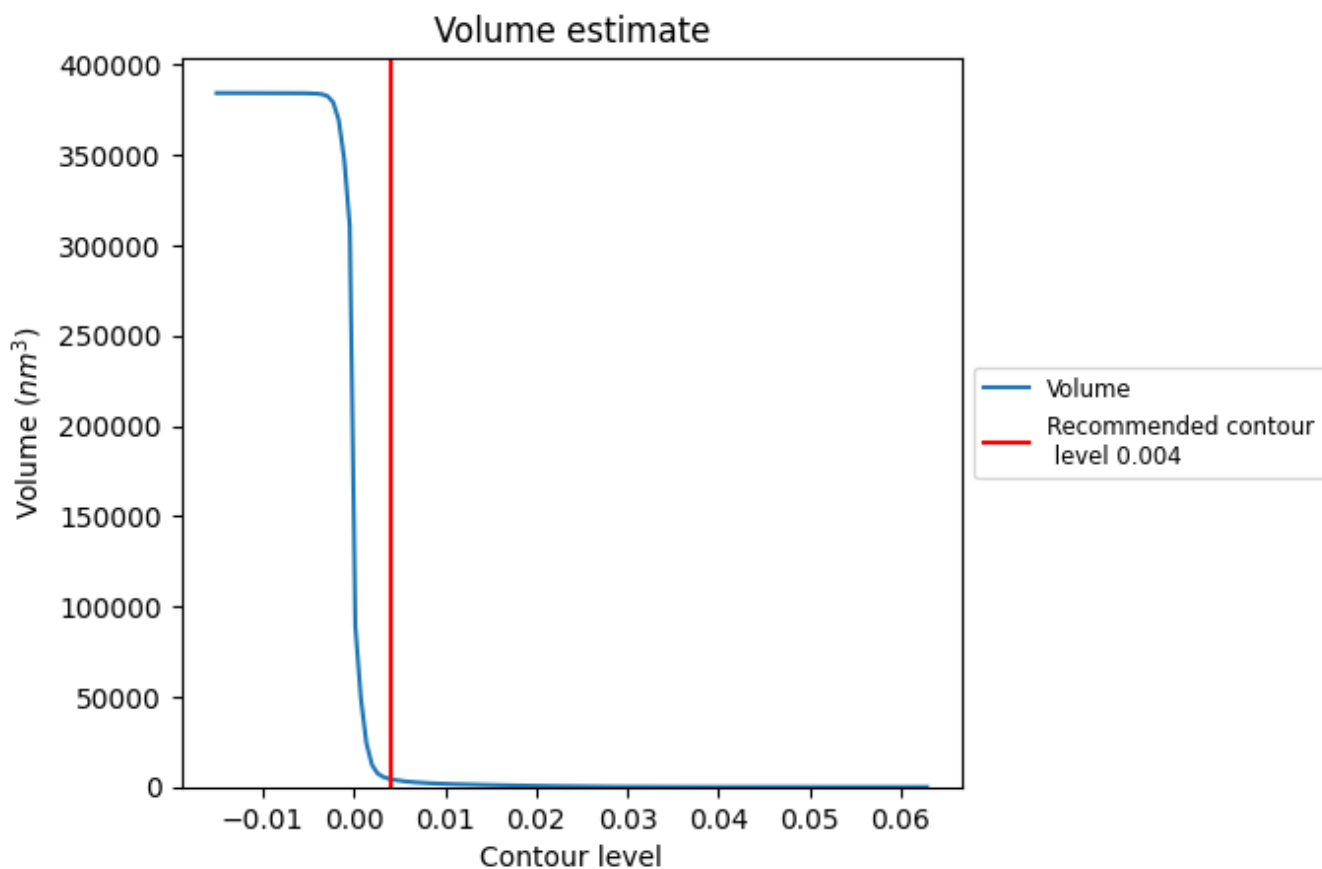
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

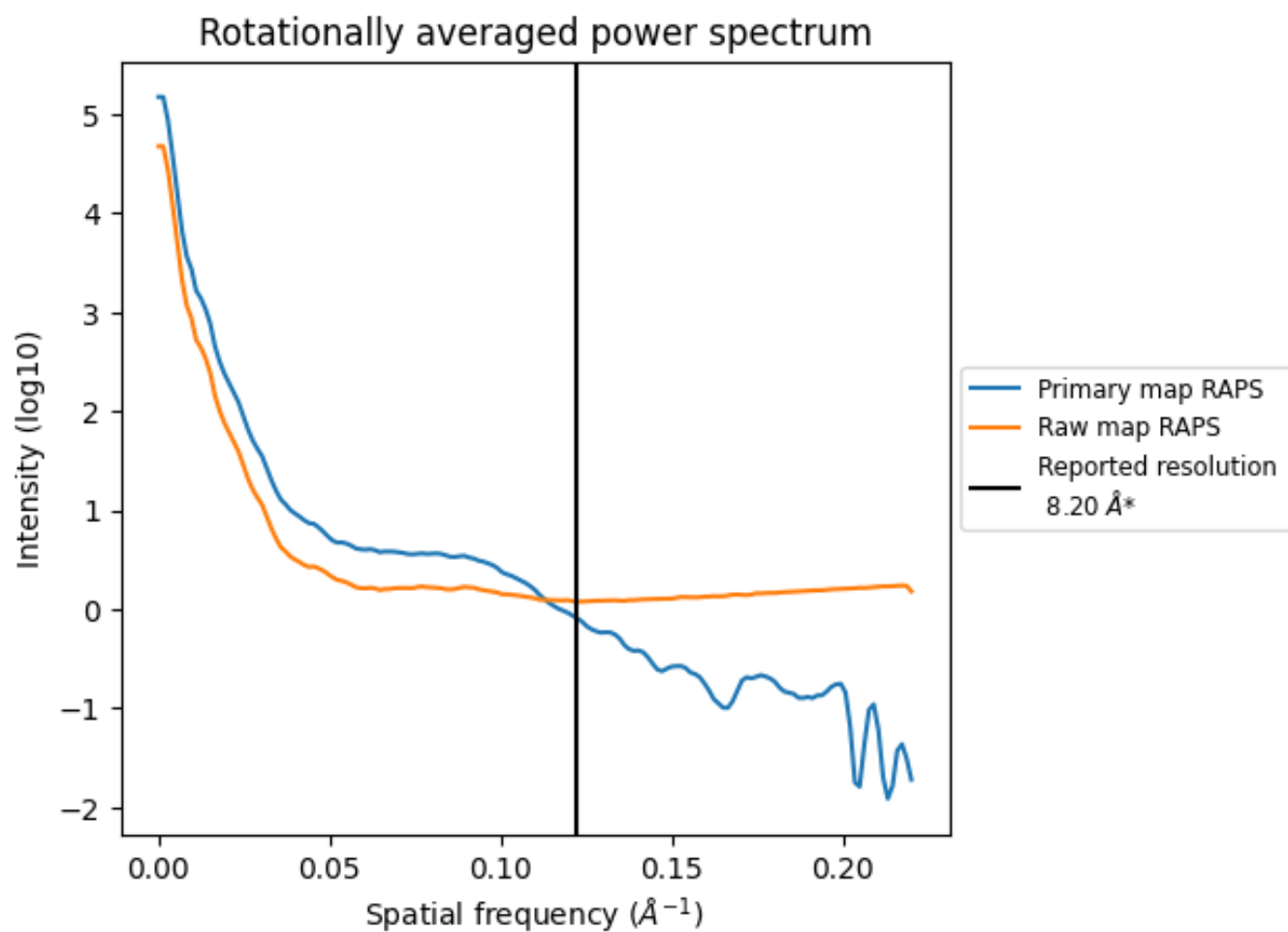
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 4396 nm<sup>3</sup>; this corresponds to an approximate mass of 3971 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i

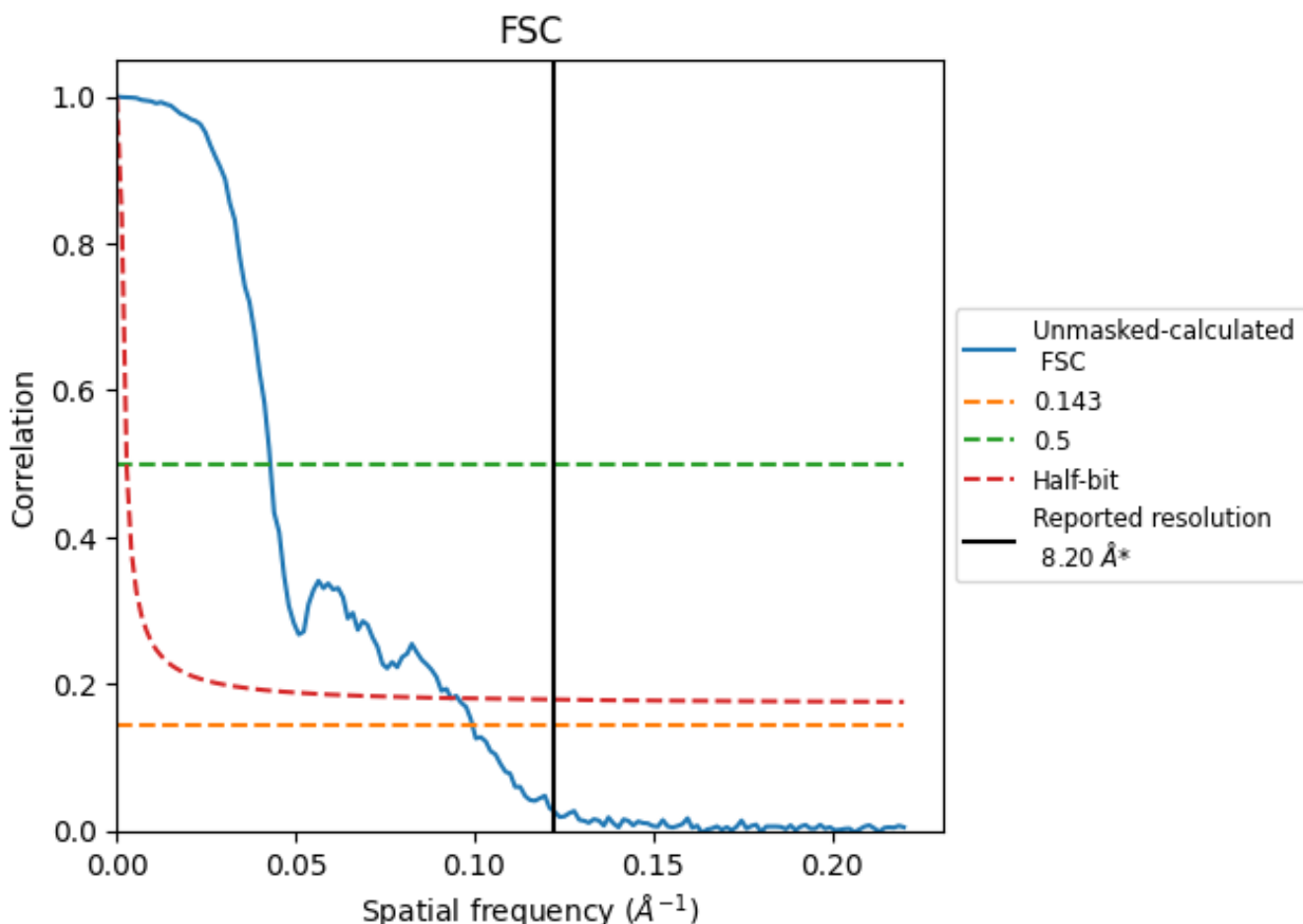


\*Reported resolution corresponds to spatial frequency of 0.122 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.122 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.05	23.31	10.70

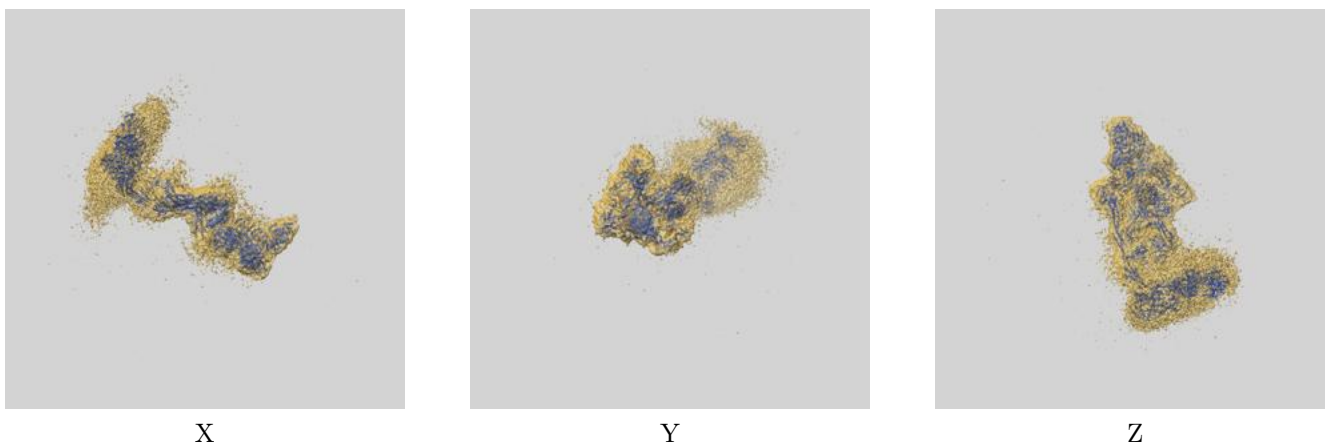
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.05 differs from the reported value 8.2 by more than 10 %



## 9 Map-model fit [i](#)

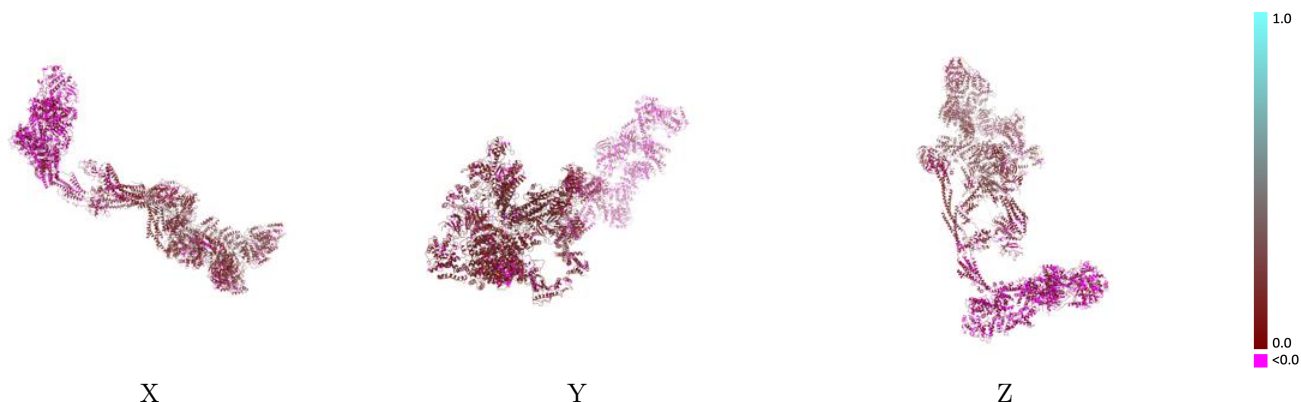
This section contains information regarding the fit between EMDB map EMD-41565 and PDB model 8TQW. Per-residue inclusion information can be found in section [3](#) on page [9](#).

### 9.1 Map-model overlay [i](#)



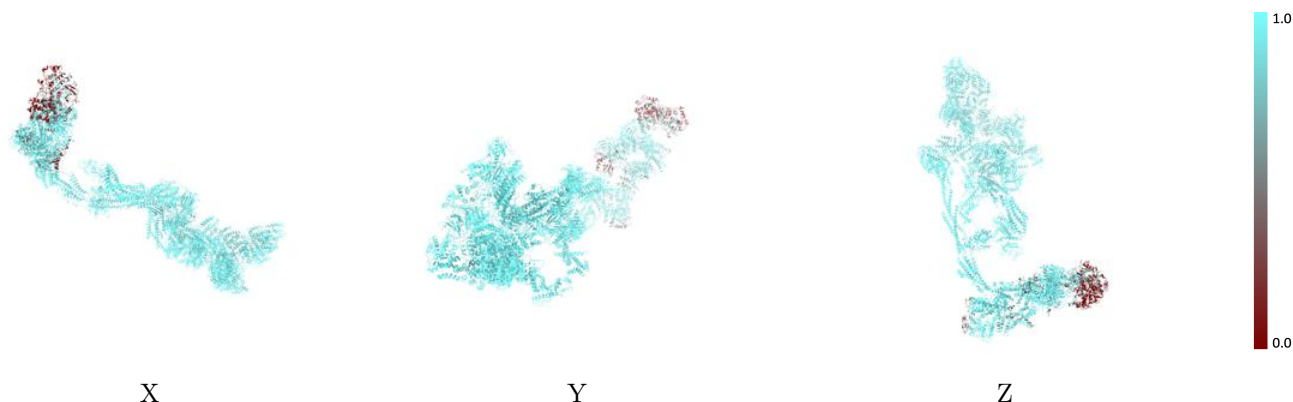
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



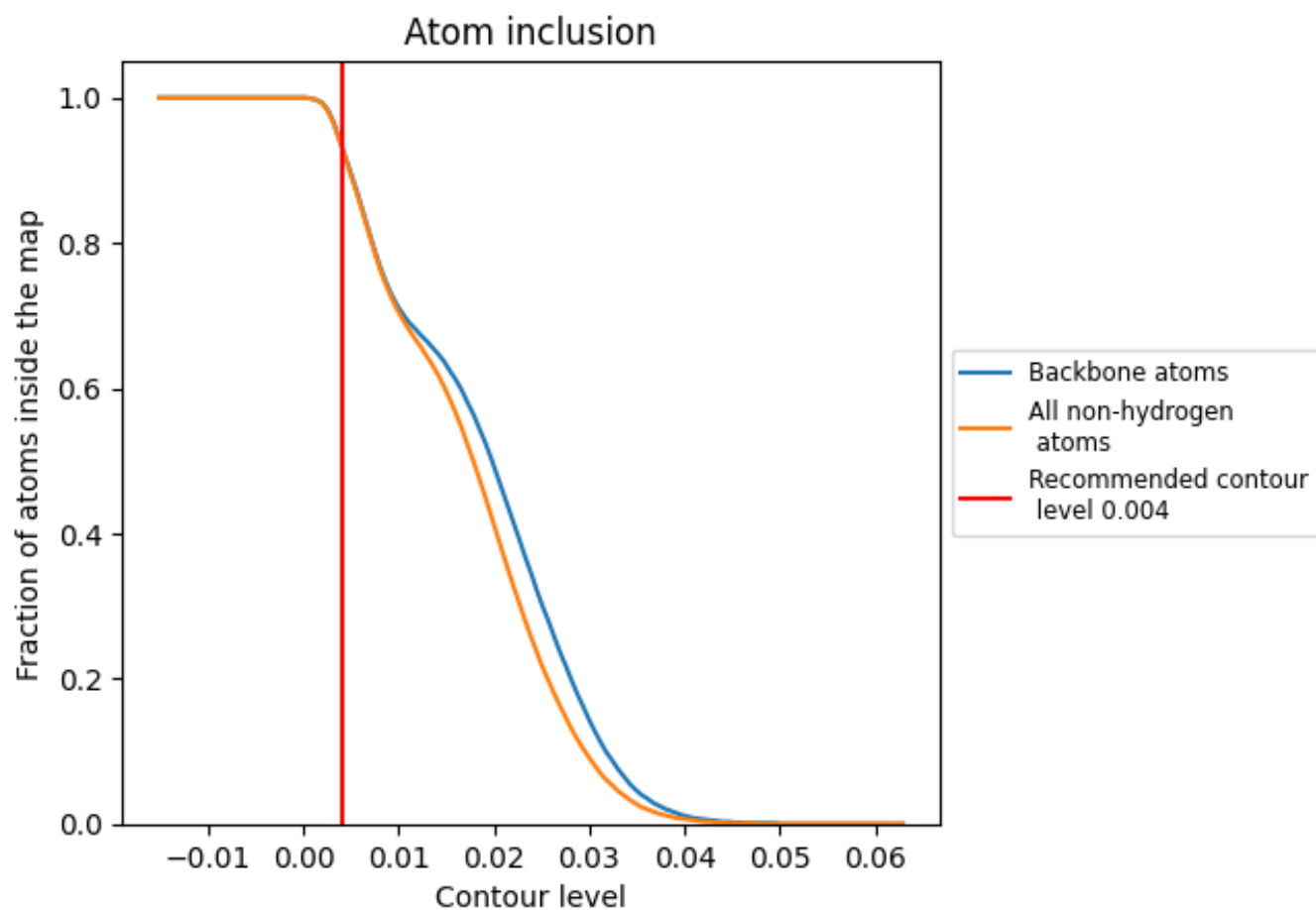
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).





























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.1110
0	 0.9980	 0.1790
1	 1.0000	 0.1670
2	 1.0000	 0.1470
3	 1.0000	 0.1610
4	 1.0000	 0.0940
A	 1.0000	 0.1290
B	 1.0000	 0.2460
D	 1.0000	 0.1340
F	 1.0000	 0.0940
G	 0.9990	 0.0980
H	 0.9950	 0.1220
I	 1.0000	 0.1670
J	 0.9960	 0.0370
K	 1.0000	 0.1270
N	 1.0000	 0.1720
O	 1.0000	 0.2010
P	 0.9990	 0.1450
Q	 1.0000	 0.1780
R	 1.0000	 0.1390
S	 1.0000	 0.0690
T	 1.0000	 0.1490
U	 0.9960	 0.0850
V	 1.0000	 0.1440
W	 1.0000	 0.1550
X	 0.9990	 0.1660
a	 0.3260	 0.0050
b	 0.2570	 0.0040
c	 0.8820	 0.0110
d	 0.8920	 0.0170

